

2,2,3-Trimethylbutane
464-06-2 | DTXSID7060047

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 92.7 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.17e-01

Confidence level: 8.17e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Carbonyl sulfide</div> <div>Measured: 102</div> <div>Predicted: 6840</div>	<div>Image not found</div> <div>3,6-Diacetylmorphine</div> <div>Measured: 82.7</div> <div>Predicted: 1.04e-09</div>	<div>Image not found</div> <div>1-Chloropropene</div> <div>Measured: 105</div> <div>Predicted: 345</div>
<div>Image not found</div> <div>Ethane, 1,2-dibromo-1,1-dichloro-</div> <div>Measured: 319</div> <div>Predicted: 1.55</div>	<div>Image not found</div> <div>1,1-Dichloro-1-nitroethane</div> <div>Measured: 20.9</div> <div>Predicted: 11.0</div>	